

1. "A Method for Describing Resonance Between Generalized Valence Bond Wavefunctions," Arthur F. Voter and William A. Goddard, III, *Chem. Phys.* **57**, 253 (1981).
2. "The Generalized Resonating Valence Bond Method: Barrier Heights in the $HF + D$ and $HCl + D$ Exchange Reactions", Arthur F. Voter and William A. Goddard, III, *J. Chem. Phys.* **75**, 3638 (1981).
3. "Transition State Theory Description of Surface Self-Diffusion: Comparison with Classical Trajectory Results," Arthur F. Voter and Jimmie D. Doll, *J. Chem. Phys.* **80**, 5832 (1984).
4. "Surface Self-Diffusion Constants at Low Temperature: Monte Carlo Transition State Theory with Importance Sampling," Arthur F. Voter and Jimmie D. Doll, *J. Chem. Phys.* **80**, 5814 (1984).
5. "Dynamical Corrections to Transition State Theory for Multistate Systems: Surface Self-Diffusion in the Rare-Event Regime," Arthur F. Voter and Jimmie D. Doll, *J. Chem. Phys.* **82**, 80 (1985).
6. "A Monte Carlo Method for Determining Free-Energy Differences and Transition State Theory Rate Constants," Arthur F. Voter, *J. Chem. Phys.* **82**, 1890 (1985).
7. "The Isotope and Temperature Dependence of the Self-Diffusion for Hydrogen, Deuterium, and Tritium on Cu(100) in the 100-1000 K Range," Steven M. Valone, Arthur F. Voter, and Jimmie D. Doll, *Surface Science* **155**, 687 (1985).
8. "Intraatomic Exchange and the Violation of Hund's Rule in Twisted Ethylene," Arthur F. Voter, Marvin M. Goodgame, and William A. Goddard, III, *Chem. Phys.* **98**, 7 (1985).
9. "The Resonating Valence Bond Description of Cyclobutadiene," Arthur F. Voter and William A. Goddard, III, *J. Am. Chem. Soc.* **108**, 2831 (1986).
10. "Summary Abstract: A New Approach to Overlayer Dynamics," Arthur F. Voter, *J. Vac. Sci. Technol. A* **4**, 1528 (1986).
11. "Testing Site Size Requirements in Chemisorption: Experiment and Theory," Charles T. Campbell, Mark T. Paffett, and Arthur F. Voter, *J. Vac. Sci. Technol. A* **4**, 1342 (1986).
12. "Oscillatory Surface Relaxations in Ni, Al, and Their Ordered Alloys," S.P. Chen, A. F. Voter, and D. J. Srolovitz, *Phys. Rev. Lett.* **57**, 1308 (1986).
13. "Computer Simulation of Grain Boundaries in Ni_3Al : The Effect of Grain Boundary Composition," S.P. Chen, A. F. Voter, and D. J. Srolovitz, *Scripta Met.* **20**, 1389 (1986).
14. "Classically Exact Overlayer Dynamics: Diffusion of Rhodium Clusters on Rh(100)," Arthur F. Voter, *Phys. Rev. B* **34**, 6819 (1986).
15. "The Influence of Substrate Motion on the Self-Diffusion of Hydrogen and its Isotopes on the Copper (100) Surface," S.M. Valone, A.F. Voter, and J.D. Doll, *J. Chem. Phys.* **85**, 7480 (1986).
16. "Accurate Interatomic Potentials for Ni, Al, and Ni_3Al ," Arthur F. Voter and Shao Ping Chen, *Mat. Res. Soc. Symp. Proc.* **82**, 175 (1987). (Winter MRS Meeting, Boston, MA, December 1986)

17. "Atomistic Simulations of Surface Relaxations in Ni, Al, and Their Ordered Alloys," S.P. Chen, A.F. Voter and D.J. Srolovitz, Mat. Res. Soc. Symp. Proc. **82**, 515 (1987). (Winter MRS Meeting, Boston, MA, December 1986)
18. "Atomistic Simulations of [001] Symmetric Tilt and Boundaries in Ni_3Al ," S.P. Chen, A.F. Voter, and D.J. Srolovitz, Mat. Res. Soc. Symp. Proc. **81**, 45 (1987). (Winter MRS Meeting, Boston, MA, December 1986)
19. "Recent Developments in the Theory of Surface Diffusion," J.D. Doll and A.F. Voter, Ann. Rev. Phys. Chem. **38**, 413 (1987).
20. "Simulation of the Layer-Growth Dynamics in Silver Films: Dynamics of Adatom Clusters and Vacancy Clusters on Ag(100)," A.F. Voter, in Modeling of Optical Thin Films, M.R. Jacobson, Ed., Proc. SPIE **821**, 214 (1987). (Proceedings of SPIE Meeting, San Diego, August 1987)
21. "A Simulation Study of Interfaces in Ni, Al, and Ni_3Al With and Without Boron," S.P. Chen, A.F. Voter and D.J. Srolovitz, Journal de Physique **49**, C5-157 (1988). (Conference on Interface Science and Engineering, Lake Placid, New York, July 21-17, 1987)
22. "Recent Developments in the Theory of Many-Body Processes: Implications for the Study of Surface Dynamics," J.D. Doll, D.L. Freeman and A.F. Voter, in Diffusion at Interfaces: Microscopic Concepts, M. Grunze, H.J. Kruezer, and J.J. Weimer, Eds., (Springer Verlag, 1988). (Proc. of the 2nd Campobello Island Surface Science Conference, Canada, August 1987)
23. "Oscillatory Relaxations in (111) Planar Defects in Ni_3Al ," D. Farkas, E.J. Savino, P. Chidambaram, A.F. Voter, D.J. Srolovitz, and S.P. Chen, Phil. Mag. A **60**, 433 (1989).
24. "Computer Simulation on Surfaces and [001] Symmetric Tilt Boundaries in Ni, Al and Ni_3Al ," S.P. Chen, D.J. Srolovitz and A.F. Voter, J. Mat. Res. **4**, 62 (1989).
25. "Structure of Grain Boundaries in Iron," R.J. Harrison, F. Spaepen, A.F. Voter and S.P. Chen, in "Innovations in Ultra high-Strength Steel Technology," G. B. Olson, M. Azrin, and E. S. Wright, Eds., Proceedings of the 34th Sagamore Army Materials Research Conference, August 31-September 3, 1987, Lake George, New York, p. 651.
26. "Theoretical Studies of Grain Boundaries in Ni, Al, and Ni_3Al with and without Boron," S.P. Chen, A.F. Voter, R.C. Albers, A.M. Boring, and P.J. Hay, Mat. Res. Symp. Proc. **122**, 355 (1988). (MRS Meeting, Reno, Nevada, April 7-9, 1988)
27. "Interference of Surface Relaxations in Unsupported Thin Films," S.P. Chen, A.F. Voter and R.C. Albers, Phys. Rev. B **39**, 1395 (1989).
28. "Computing Classically Exact Diffusion Constants Using Short Time Trajectories," A.F. Voter, Phys. Rev. Lett. **63**, 167 (1989).
29. "Classically Exact Surface Diffusion Constants at Arbitrary Temperature," A.F. Voter and J.M. Cohen, J. Vac. Sci. Tech. A **7**, 1859 (1989). (Proceedings of October 1988 AVS Meeting, Atlanta, GA)
30. "Using Multistate Dynamical Corrections to Compute Classically Exact Diffusion Constants at Arbitrary Temperature," A.F. Voter, J.D. Doll, and J.M. Cohen, J. Chem. Phys. **90**, 2045 (1989).
31. "Theoretical Studies of Grain Boundaries in Ni_3Al with Boron or Sulfur," S.P. Chen, A.F. Voter, R.C. Albers, A.M. Boring, and P.J. Hay, Scripta Met., **23**, 217 (1989).

32. "Grain Boundary Structure and Intergranular Fracture in $L1_2$ Ordered Alloys," V. Vitek, S.P. Chen, A.F. Voter, J.J. Kruisman, and J.Th.M. DeHosson in *Grain Boundary Chemistry and Intergranular Fracture*, G.S. Was, Ed. (Trans. Tech. Publication, 1989), *Materials Science Forum* **46**, 237 (1989).
33. "The Effects of B and S on Ni_3Al Grain Boundaries," A.F. Voter, S.P. Chen, R.C. Albers, A.M. Boring, and P.J. Hay in *Atomistic Simulation of Materials: Beyond Pair Potentials*, V. Vitek and D.J. Srolovitz, Eds., Plenum, 1989, p. 223 (Proc. of the 1988 World Materials Congress, Chicago, September 1988)
34. "Embedded Atom Potential for BCC Iron," R.J. Harrison, A.F. Voter, and S.P. Chen in *Atomistic Simulation of Materials: Beyond Pair Potentials*, V. Vitek and D.J. Srolovitz, Eds., Plenum, 1989, p. 219. (Proc. of the 1988 World Materials Congress, Chicago, September 1988)
35. "Molecular Dynamics Study of Crack Propagation in Ni-Al," S. Charpenay, P.C. Clapp, J.A. Rifkin, Z.Z. Yu, and A.F. Voter in *Mat. Res. Soc. Symp. Proc.* **141**, 323 (1989).
36. "Some Thermodynamics Properties of NiAl Calculated by Molecular Dynamics Simulations," P.C. Clapp, M.J. Rubins, S. Charpenay, J.A. Rifkin, Z.Z. Yu, and A.F. Voter in *Proc. of the MRS Fall Meeting*, Boston, MA, November 28 - December 3, 1988.
37. "Theoretical Studies of Ni_3Al and NiAl with Impurities," S.P. Chen, A.F. Voter, A. M. Boring, R.C. Albers, and P. J. Hay, *Mat. Res. Soc. Symp. Proc.*, **133**, 149 (1989). (Winter MRS meeting, Boston, MA, 1988)
38. "Self-Diffusion on the Lenard-Jones FCC(111) Surface: Effects of Temperature on Dynamical Corrections," J.M. Cohen and A.F. Voter, *J. Chem. Phys.* **91**, 5082 (1989).
39. "Investigation of the Effects of Boron on Ni_3Al Grain Boundaries by Atomistic Simulations," S. P. Chen, A. F. Voter, R. C. Albers, A. M. Boring, and P. J. Hay, *J. Mater. Res.* **5**, 955 (1990).
40. "Reconstruction of the (310), (210), and (110) Surfaces in FCC Metals," S. P. Chen and A. F. Voter, *Surf. Sci. Lett.* **244**, L107 (1991).
41. "EAM Study of Surface Self-Diffusion of Single Adatoms of FCC Metals Ni, Cu, Al, Ag, Au, Pd, and Pt," C. L. Liu, J. M. Cohen, J. B. Adams, and A. F. Voter, *Surf. Sci.*, **253**, 334 (1991).
42. "Interatomic Potential for Directional Bonding: The Rotated Second Moment Approximation," J. D. Kress and A. F. Voter, *Phys. Rev. B* **43**, 12607 (1991).
43. "Effects of Pairwise Versus Many-Body Forces on High-Stress Plastic Deformation," B. L. Holian, A. F. Voter, N. J. Wagner, R. J. Ravelo, S. P. Chen, W. G. Hoover, C. G. Hoover, J. E. Hammerberg, and T. D. Dontje, *Phys. Rev. A*, **43**, 2655 (1991).
44. "Surface Diffusion Modes for Pt Dimers and Trimers on Pt(001)," G. L. Kellogg and A. F. Voter, *Phys. Rev. Lett.* **67**, 622 (1991).
45. "Model Description of Transition Metals Using the Rotated Second Moment Approximation," J. D. Kress and A. F. Voter, *Radiation Effects and Defects in Solids*, **129**, 45 (1994). (Proceedings of the 1991 IEA Workshop on the Use of Molecular Dynamics in Modeling Radiation Effects and Other Non-Equilibrium Phenomena).
46. "Phase Changes in Nickel Clusters from an Embedded-Atom Potential," Z. B. Güvenç, J. Jellinek, and A. F. Voter, *Physics and Chemistry of Finite Systems: From Clusters to Crystals*, Vol I, 411 (Kluwer Academic Publishers, Netherlands, 1992).

47. "Molecular Dynamics Simulations of Two-dimensional Materials at High Strain Rates," N. J. Wagner, B. L. Holian, and A. F. Voter, Phys. Rev. A **45**, 8457 (1992).
48. "The Embedded Atom Method," A. F. Voter, in "Intermetallic Compounds: Principles and Practice," edited by J.H. Westbrook and R.L. Fleischer, John Wiley and Sons, Ltd, 1995, p. 77.
49. "Atomistic Simulation of Diamond-Tip Machining of Nanoscale Features," Arthur F. Voter and Joel D. Kress, Proceedings of the American Society of Precision Engineering (ASPE) conference, Tucson, AZ, April 1993.
50. "Convergence of Surface Diffusion Parameters with Model Crystal Size," Jennifer M. Cohen and Arthur F. Voter, Surf. Sci., **313**, 439 (1994).
51. "Atomistic Study of Energy and Structure of Surfaces in NiO," M. Yan, S.P. Chen, A.F. Voter, and T.E. Mitchell, in *Structure and Properties of Interfaces in Ceramics*, ed. by D. Bonnell, U. Chowdhry and M. Ruhle, Mat. Res. Symp. Proc. Vol. 357, p. 441, (1995).
52. "Interatomic Potentials from Tight-Binding Moment Expansions," J.D. Kress and A.F. Voter, Phys. Rev. B **52**, 8766 (1995).
53. "Polynomial Approximations for Materials Simulations," R.N. Silver, A.F. Voter, J.D. Kress, and H. Roeder, Simulation MultiConference '95 Proceedings, High Performance Computing '95, edited by A. Tentner, p. 200 (1995).
54. "Kernel Polynomial Approximations for Densities of States and Spectral Functions," R.N. Silver, H. Roeder, A.F. Voter and J.D. Kress, J. Comp. Phys. **124**, 115 (1996). (Figure 4 of this paper was used on the cover of the issue).
55. "Interatomic Potentials for Covalent Materials from a Local Approximation to Tight Binding," A.F. Voter, J.D. Kress, and R.N. Silver, Proceedings of Computational Modelling of Materials and Processing Symposium, 97th Annual Meeting of the American Ceramics Society, Cincinnati, OH 1995.
56. "Thermostatted molecular dynamics: How to avoid the Toda demon hidden in Nose-Hoover dynamics," B.L. Holian, A.F. Voter, and R. Ravelo, Phys. Rev. E, **52**, 2338 (1995).
57. "Linear-scaling Tight Binding from a Truncated Moment Approach," A.F. Voter, J.D. Kress, and R.N. Silver, Phys. Rev. B **53**, 12733 (1996).
58. "Chebyshev Recursion Methods: Kernel Polynomials and Maximum Entropy," R.N. Silver, H. Roeder, A.F. Voter, and J.D. Kress, in International Symposium on Coherent Approaches to Fluctuations, eds. M. Suzuki, N. Kawashima, World Scientific, Singapore, p. 119-124 (1996). (proceedings of Hayashibara Forum '95, International Symposium on Coherent Approaches to Fluctuations, Kyoto, Japan, July 1995.)
59. "Electrically Inactive Poly-Silicon Grain Boundaries," S.P. Chen, J.D. Kress, A.F. Voter and R.C. Albers, Electrochemical Society Series, **96**, 359 (1996).
60. "Interatomic Potentials for Materials Simulation: Progress and Perspectives," *MRS Bulletin*, edited by A.F. Voter, **21**, 17 (1996).
61. "Efficient Maximum Entropy Algorithms for Electronic Structure," R.N. Silver, H. Roeder, A.F. Voter and J.D. Kress, Simulation MultiConference '96 Proceedings, High Performance Computing '96, edited by xxx, page xxx (1996).

62. "Highly optimized tight-binding model of silicon," T.J. Lenosky, J.D. Kress, I. Kwon, A.F. Voter, B. Edwards, D.F. Richards, S. Yang, and J.B. Adams, Phys. Rev. B **55**, 1528 (1997).
63. "A method for accelerating the molecular dynamics simulation of infrequent events," A.F. Voter, J. Chem. Phys. **106**, 4665 (1997).
64. "Dislocation emission from a three-dimensional crack – a large-scale molecular dynamics study," S.J. Zhou, D.M. Beazley, P.S. Lomdahl, A.F. Voter, and B.L. Holian, Advances in Fracture Research, Vols. 1-6, p. 3085 (1997). (Proceedings of the 9th International Conference on Fracture (Sydney, April 1-5, 1997)
65. "Hyperdynamics: Accelerated Molecular Dynamics of Infrequent Events," A.F. Voter, Phys. Rev. Lett. **78**, 3908 (1997).
66. "Accelerated Molecular Dynamics of Materials Defects with the Hyper-MD Method," A.F. Voter, in *Novel Materials*, edited by B. K. Rao and S. N. Behera (Nova Scientific, New York, 1997). (Proceedings of the International Symposium on Novel Materials, Puri, India, March 3-7, 1997)
67. "Influence of the local microstructure on the macroscopic properties of $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$," W. Windl, J.D. Kress, A.F. Voter, J. Menendez, and O.F. Sankey, Mat. Res. Soc. Symp. Proc. **469**, 433 (1997)
68. "Molecular Dynamics Simulation of Reactive Ion Etching of Si by Energetic Cl Ions," D.E. Hanson, A.F. Voter, and J.D. Kress, J. Appl. Phys. **82**, 3552 (1997).
69. "First-Principles Calculation of Displacement-Threshold Energies in Si and SiC," W. Windl, T.J. Lenosky, J.D. Kress, and A.F. Voter, Nuclear Instruments and Methods in Physics Research B, **141**, 61 (1998).
70. "Atomistic Simulation Methods," A. F. Voter, in Morphological Organizations in Epitaxial Growth and Removal, p. 30 (World Scientific, 1997).
71. "An Interatomic Potential for Reactive Ion Etching of Si by Cl Ions," D.E. Hanson, J.D. Kress, and A.F. Voter, J. Chem. Phys. **110**, 5983 (1999).
72. "Parallel Replica Method for Dynamics of Infrequent Events," A.F. Voter, Phys. Rev. B **57**, R13985 (1998).
73. "Molecular dynamics-based ion-surface interaction models for ionized physical vapor deposition feature scale simulations," D.G. Coronell, D.E. Hanson, A.F. Voter, C.L. Liu, X.-Y. Liu, and J.D. Kress, Appl. Phys. Lett. **73**, 3860 (1998).
74. "Molecular dynamics Simulations of Cu and Ar Ion Sputtering of Cu(111) Surfaces," J.D. Kress, D.E. Hanson, A.F. Voter, C.L. Liu, X.-Y. Liu, and D.G. Coronell, J. Vac. Sci. Tech. A **17**, 2819 (1999).
75. "Reactive Ion Etching of Si by Cl, Cl_2 and Ar Ions: Molecular Dynamics Simulations with Comparisons to Experiment" D.E. Hanson, J.D. Kress, and A.F. Voter, J. Vac. Sci. Tech. A **17**, 1510 (1999).
76. "Self-Diffusion Within the Cores of a Dissociated Glide Dislocation in an FCC Solid," R.G. Hoagland, A.F. Voter, and S.M. Foiles, Scripta. Met. **39**, 589 (1998).
77. "Three-dimensional fracture via large-scale molecular dynamics," S.J. Zhou, P.S. Lomdahl, A.F. Voter, and B.L. Holian, Engineering Fracture Mechanics **61**, 173 (1998).

78. "Accelerating the Dynamics of Infrequent Events: Combining Hyperdynamics and Parallel Replica Dynamics to Treat Epitaxial Layer Growth," A.F. Voter and T.C. Germann, Mat. Res. Soc. Symp. Proc. **528**, 221 (1998). (proceedings of 1998 Spring MRS meeting)
79. "Bias Potentials for Hyperdynamics Simulations" W.G. Rudd and A.F. Voter, Mat. Res. Soc. Symp. Proc. **538**, 485 (1999). (proceedings of 1998 Fall MRS meeting)
80. "Accelerating Atomistic Simulations of Defect Dynamics: Hyperdynamics, Parallel Replica Dynamics, and Temperature-Accelerated Dynamics," A.F. Voter and M.R. Sørensen, Mat. Res. Soc. Symp. Proc. **538**, 427 (1999). (proceedings of 1998 Fall MRS meeting)
81. "Temperature Accelerated Dynamics for Simulation of Infrequent Events," M.R. Sørensen and A.F. Voter, J. Chem. Phys. **112**, 9599 (2000).
82. "Trapping and Desorption of Energetic Cu atoms on Cu(111) and (001) Surfaces at Grazing Incidence," D.E. Hanson, J.D. Kress, A.F. Voter, and X.-Y. Liu, Phys. Rev. B **60**, 11723 (1999).
83. "Dimensional Strategies and the Minimization Problem: Barrier-Avoiding Algorithms," D.B. Faken, A.F. Voter, D.L. Freeman and J.D. Doll, J. Phys. Chem. **A103**, 9521 (1999).
84. "Compact Surface Cluster Diffusion by Concerted Rotation and Translation?," J.C. Hamilton, M.R. Sørensen, and A.F. Voter, Phys. Rev. B **61**, R5125 (2000).
85. "Highly Optimized Empirical Potential Model of Silicon," T.J. Lenosky, B. Sadigh, E. Alonso, V.V. Bulatov, T. Diaz de la Rubia, J. Kim, A.F. Voter and J.D. Kress, Modelling and Simulation in Materials Science and Engineering, **8**, 825 (2000).
86. "Diffusion Mechanisms in Cu Grain Boundaries," Y. Mishin, M.R. Sørensen, and A.F. Voter, Phys. Rev. B **62**, 3658 (2000).
87. "Atomic Mechanisms of Grain Boundary Diffusion," Y. Mishin, M.R. Sørensen, and A.F. Voter, in *Mass and Charge Transfer in Inorganic Materials: Fundamentals to Devices*, edited by P. Vincenzini and V. Buscaglia, Faenza (2000), Techna Srl, p. 377. (Venice workshop proceedings)
88. "Failure of 1D Models for Ir Island Diffusion on Ir(111)," J.C. Hamilton and A.F. Voter, Phys. Rev. Lett. **85**, 1580 (2000). (Comment)
89. "Calculation of Point-Defect Entropy in Metals," Y. Mishin, M.R. Sørensen, and A.F. Voter, Phil. Mag. A., **81**, 2591 (2001).
90. "Smart Darting Monte Carlo" I. Andricioaei, J.E. Straub, and A.F. Voter, J. Chem. Phys. **114**, 6994 (2001).
91. "Structural stability and lattice defects in copper: Ab initio, tight-binding, and embedded-atom calculations" Y. Mishin, M.J. Mehl, D.A. Papaconstantopoulos, A.F. Voter, and J.D. Kress, Phys. Rev. B **63**, 224106 (2001).
92. "Normal-Incidence Steering Effect in Crystal Growth: Ag/Ag(100)" F. Montalenti and A.F. Voter, Phys. Rev. B **64**, 081401(R) (2001).
93. "Applying Accelerated Molecular Dynamics to Crystal Growth" F. Montalenti and A.F. Voter, Phys. Stat. Sol. (B) **226**, 21 (2001).
94. "Accelerated dynamics simulations of interstitial-cluster growth," S. Birner, J. Kim, D.A. Richie, J.W. Wilkins, A.F. Voter, and T. Lenosky, Solid State Comm. **120**, 279 (2001).

95. "Closing the Gap Between Experiment and Theory: Crystal Growth by Temperature Accelerated Dynamics" F. Montalenti, M.R. Sørensen, and A.F. Voter, Phys. Rev. Lett., **87**, 126101 (2001).
96. "Exploiting past visits or minimum-barrier knowledge to gain further boost in the temperature-accelerated dynamics method" F. Montalenti and A.F. Voter, J. Chem. Phys. **116**, 4819 (2002).
97. "Extending the Time Scale in Atomistic Simulation of Materials," A.F. Voter, F. Montalenti and T.C. Germann, Annu. Rev. Mater. Res. **32**, 321 (2002).
98. "Application of parallel replica dynamics to pyrolysis of n-hexadecane," O. Kum, B.M. Dickson, S.J. Stuart, B.P. Uberuaga, and A.F. Voter, Parallel and Distributed Computing and Systems, edited by S.G. Akl and T. Gonzalez (Acta Press, Anaheim, CA, 2002) p. 507. (conference proceedings paper)
99. "Spontaneous atomic shuffle in flat terraces: Ag(100)," F. Montalenti, A.F. Voter and R. Ferrando, Phys. Rev. B **66**, 205404 (2002).
100. "Simulation of Growth of Cu on Ag(001) at Experimental Deposition Rates," J.A. Sprague, F. Montalenti, B.P. Uberuaga, J.D. Kress, and A.F. Voter, Phys. Rev. B **66**, 205415 (2002).
101. "Ion solid surface interactions in ionized copper physical vapor deposition," X.-Y. Liu, M.S. Daw, J.D. Kress, D.E. Hanson, V. Arunachalam, D.G. Coronell, C.-L. Liu, and A.F. Voter, Thin Solid Films, **422**, 141 (2002).
102. "Mechanisms and Rates of Interstitial H₂ Diffusion in Crystalline C₆₀," B.P. Uberuaga, A.F. Voter, K.K. Sieber, and D.S. Sholl, Phys. Rev. Lett. **91**, 105901-1 (2003).
103. "Accelerated molecular dynamics study of vacancies in Pu," B.P. Uberuaga, S.M. Valone, M.I. Baskes, and A.F. Voter, AIP Conference proceedings **673**, 213 (2003). (proceedings of the 3rd Topical Conference on Plutonium and Actinides, July 6-10, 2003, Albuquerque, NM)
104. "Structure and Mobility of Defects Formed from Collision Cascades in MgO," B.P. Uberuaga, R. Smith, A.R. Cleave, F. Montalenti, G. Henkelman, R.W. Grimes, A.F. Voter, and K.E. Sickafus, Phys. Rev. Lett. **92**, 115505 (2004).
105. "Synchronization of trajectories in canonical molecular-dynamics simulations: Observation, explanation, and exploitation," B.P. Uberuaga, M. Anghel, and A.F. Voter, J. Chem. Phys. **120**, 6363 (2004).
106. "Reactive Bond-Order Simulations Using Both Spatial and Temporal Approaches to Parallelism," S.J. Stuart, Y. Li, O. Kum, J.W. Mintmire, and A.F. Voter, Structural Chemistry **15**, 479 (2004).
107. "Parallel Replica Dynamics with a Heterogeneous Distribution of Barriers: Application to *n*-Hexadecane Pyrolysis," O. Kum, B.M. Dickson, S.J. Stuart, B.P. Uberuaga, and A.F. Voter, J. Chem. Phys. **121**, 9808 (2004).
108. "Exploring long-time response to radiation damage in MgO," B.P. Uberuaga, R. Smith, A.R. Cleave, G. Henkelman, R.W. Grimes, A.F. Voter, and K.E. Sickafus, Nucl. Inst. and Meth. B **228**, 260 (2005).
109. "Dynamical simulations of radiation damage and defect mobility in MgO," B.P. Uberuaga, R. Smith, A.R. Cleave, G. Henkelman, R.W. Grimes, A.F. Voter, and K.E. Sickafus, Phys. Rev. B **71**, 104102 (2005).

110. "Diffusion of small self-interstitial clusters in silicon: temperature-accelerated tight-binding molecular dynamics simulations," M. Cogoni, B.P. Uberuaga, A.F. Voter and L. Colombo, Phys. Rev. B **71**, 121203 (2005).
111. "Accelerated molecular dynamics methods," B.P. Uberuaga, F. Montalenti, T.C. Germann, and A.F. Voter, in *Handbook of Materials Modeling, Part A - Methods*, edited by S. Yip (Springer, 2005), p. 629.
112. "Determining reaction mechanisms," B.P. Uberuaga and A.F. Voter, in *Handbook of Materials Modeling, Part B - Models*, edited by S. Yip (Springer, 2005), p. 1627.
113. "Atomistic study of the dissolution of small boron interstitial clusters in c-Si," M. Cogoni, A. Mattoni, B.P. Uberuaga, A.F. Voter, and L. Colombo, Appl. Phys. Lett. **87**, 191912 (2005).
114. "Introduction to the Kinetic Monte Carlo Method," A.F. Voter, in *Radiation Effects in Solids*, edited by K. E. Sickafus, E. A. Kotomin and B.P. Uberuaga (Springer, NATO Publishing Unit, Dordrecht, The Netherlands, 2007) pp. 1-23.
115. "Accelerated Molecular Dynamics Methods," B.P. Uberuaga and A.F. Voter, in *Radiation Effects in Solids*, edited by K. E. Sickafus, E. A. Kotomin and B.P. Uberuaga (Springer, NATO Publishing Unit, Dordrecht, The Netherlands, 2006) pp. 25-43.
116. "Accelerated molecular dynamics simulations of interstitial clusters in pure and Al-doped MgO," B.P. Uberuaga, R. Smith, A.R. Cleave, R.W. Grimes, A.F. Voter, and K.E. Sickafus, Nucl. Inst. Meth. Phys. B **250**, 12 (2006).
117. "Parallel-replica dynamics for driven systems: derivation and application to strained nanotubes," B.P. Uberuaga, S.J. Stuart, and A.F. Voter, J. Chem. Phys. **75**, 014301 (2007).
118. "Defect kinetics in spinels: Long-time simulations of MgAl₂O₄, MgGa₂O₄, and MgIn₂O₄," B.P. Uberuaga, D. Bacorisen, R. Smith, J.A. Ball, R.W. Grimes, A.F. Voter, and K.E. Sickafus, Phys. Rev. B **75**, 104116 (2007).
119. "Stick-slip behavior of grain boundaries studied by accelerated molecular dynamics," Y. Mishin, A. Suzuki, B.P. Uberuaga, and A.F. Voter, Phys. Rev. B **75**, 224101 (2007).
120. "Direct transformation of vacancy voids to stacking fault tetrahedra," B.P. Uberuaga, R.G. Hoagland, A.F. Voter, and S.M. Valone, Phys. Rev. Lett. **99**, 135501 (2007).
121. "Structure and mobility of radiation-induced defects in MgO," B.P. Uberuaga, A.F. Voter, K.E. Sickafus, A. Cleave, R. Grimes, D. Bacorisen, and R. Smith, J. Computer-Aided Mater. Des. **14**, 183 (2007).
122. "Reaching extended length scales and time scales in atomistic simulations via spatially parallel temperature-accelerated dynamics," Y. Shim, J.G. Amar, B.P. Uberuaga, and A.F. Voter, Phys. Rev. B **76**, 205439 (2007).
123. "Hierarchical petascale simulation framework for stress corrosion cracking," P. Vashishta, R.K. Kalia, A. Nakano, E. Kaxiras, A. Grama, G. Lu, S. Eidenbenz, A.F. Voter, R.Q. Hood, J.A. Moriarty, and L.H. Yang, Journal of Physics Conference Series, 78, U288 (2007).
124. "Vacancy formation and strain in low-temperature Cu/Cu(100) growth," Y. Shim, V. Borovikov, B.P. Uberuaga, A.F. Voter, and J.G. Amar Phys. Rev. Lett., **101**, 116101 (2008).
125. "Accelerated Molecular Dynamics Methods: Introduction and Recent Developments," D. Perez, B.P. Uberuaga, Y. Shim, J.G. Amar, and A.F. Voter, Annual Reports in Comp. Chem. **5**, 79 (2009).

126. "Low-Speed Atomistic Simulation of StickSlip Friction using Parallel Replica Dynamics," A. Martini, Y. Dong, D. Perez, and A.F. Voter, *Tribol. Lett.*, **36**, 63 (2009).
127. "Rapid Diffusion of Magic-Size Islands by Combined Glide and Vacancy Mechanism," O.U. Uche, D. Perez, A.F. Voter, and J.C. Hamilton, *Phys. Rev. Lett.*, **103**, 046101 (2009).
128. "Bad Seeds Sprout Perilous Dynamics: Stochastic Thermostat Induced Trajectory Synchronization in Biomolecules," D.J. Sindhikara, S. Kim, A.F. Voter, and A.E. Roitberg, *J. Chem. Theory and Comp.*, **5**, 1624 (2009).
129. "Efficient annealing of radiation damage near grain boundaries via interstitial emission," X.M. Bai, A.F. Voter, R.G. Hoagland, M. Nastasi, and B.P. Uberuaga, *Science*, **327**, 1631 (2010).
130. "Accurate acceleration of kinetic Monte Carlo simulations through the modification of rate constants," A. Chatterjee and A.F. Voter, *J. Chem. Phys.* **132**, 194101 (2010).
131. "Rate theory description of atomic stick-slip friction," D. Perez, Y. Dong, A. Martini, and A.F. Voter, *Phys. Rev. B* **81**, 245415 (2010).
132. "Understanding the Surface Diffusion Processes during Magnetron Sputter-Deposition of Complex Oxide Mg-Al-O Thin Films," V. Georgieva, A.F. Voter, and A. Bogaerts, *Crystal Growth and Design* **11**, 2553 (2011).
133. "The roles of statics and dynamics in determining transitions between atomic friction regimes, Y. Dong, D. Perez, A.F. Voter, and A. Martini, *Tribology Letters* **42**, 99 (2011).
134. "Fullerene and graphene formation from carbon nanotube fragments," B.P. Uberuaga, S.J. Stuart, W. Windl, M. Masquelier, and A.F. Voter, *Computational and Theoretical Chemistry*, **987**, 115 (2012).
135. "The role of atomic structure on grain boundary-defect interactions in Cu," Xian-Ming Bai, Louis J. Vernon, Richard G. Hoagland, Arthur F. Voter, Michael Nastasi, and Blas Pedro Uberuaga, *Phys. Rev. B* **85**, 214103 (2012).
136. "Accelerated Molecular Dynamics Methods," D. Perez, B.P. Uberuaga, and A.F. Voter, in *Hierarchical Methods for Dynamics in Complex Molecular Systems*, Forshungszentrum Julich, (2012).
137. "Locally disrupted synchronization in Langevin molecular dynamics," A.I. Georgescu, S. Denny, E. Joly, G. Chen, D. Perez, and A.F. Voter, *Phys. Rev. E*, **86**, 026703 (2012).
138. "Influence of point defects on grain boundary mobility in bcc tungsten," Valery Borovikov, Xian-Zhu Tang, Danny Perez, Xian-Ming Bai, Blas P. Uberuaga, and Arthur F. Voter, *J. Phys.: Condens. Matter* **25**, 035402 (2013).

TECHNICAL REPORTS

"Embedded Atom Method Potentials for Seven FCC Metals: Ni, Pd, Pt, Cu, Ag, Au, and Al," Arthur F. Voter, Los Alamos Unclassified Technical Report # LA-UR-93-3901 (1993).